

Borel Summation Method and First Order Perturbation Formula for the Potential $V(r) = F/r^2 + G/r + H/(r + z^2)$

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The Borel Summation Method is applied to obtain a first order formula for the bound states for the potential $V(r) = F/r^2 + G/r + H/(r + z^2)$. For small H our formula reproduces the numerical results given by Znojil.

1. Introduction

The modified Coulomb potential

$$V(r) = F/r^2 + G/r + H/(r + z^2),$$

represents a simple model of Coulomb screening and hence is of some interest in atomic and molecular physics. Recently Znojil [1] discussed this potential and related it to the case of the anharmonic oscillator problem of the type [2]

$$V(x) = x^2 + \lambda x^2/(1 + g x^2).$$

But this approach does not give any direct formula for the energy eigenvalues. He also discussed the solution in the framework of continued fractions, which can be used to find the bound states numerically.

In this note we show that an exact first order perturbation formula exists for this potential which for small H accurately reproduces the eigenvalues obtained by numerical methods. This formula is obtained by using Borel's summation method after Popov et al. [3].

2. Schrödinger Equation and Perturbation Method

The Schrödinger equation with the potential

$$V(r) = \frac{F}{r^2} + \frac{G}{r} + \frac{H}{r + z^2}$$

is

$$\left\{ -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{F}{r^2} + \frac{G}{r} + \frac{H}{r+z^2} \right\} \psi(r) = E \psi(r) \quad (1)$$

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(we use the units $m = \hbar = c = 1$). Equation (1) can be put in the form

$$\left\{ \frac{d^2}{dr^2} + E - \frac{G}{r} - \frac{L(L+1)}{r^2} - \frac{H}{r+z^2} \right\} \psi(r) = 0, \quad (2)$$

where

$$L(L+1) = l(l+1) + F. \quad (3)$$

Treating the term $H/(r+z^2)$ as the perturbation term, the unperturbed equation reduces to

$$\left\{ \frac{d^2}{dr^2} + E - \frac{G}{r} - \frac{L(L+1)}{r^2} \right\} \psi(r) = 0, \quad (4)$$

which is the eigenvalue equation for the Hydrogen atom in a Coulomb potential (see for example Flügge [4]).

The eigenfunctions for (4) are given by

$$\psi(r) = \left[\frac{\left(-\frac{G}{L+1+n_r} \right)^{2L+3} (n_r)!}{(2L+2+2n_r) [\Gamma(n_r+2L+2)]^3} \right]^{1/2} \cdot r^{L+1} \exp \left\{ \frac{Gr}{2L+2+2n_r} \right\} L_{n_r}^{2L+1} \left(-\frac{Gr}{L+1+n_r} \right), \quad (5)$$

where $n_r = 0, 1, 2, \dots$ and $L_{n_r}^{2L+1}(x)$ are associated Laguerre polynomials [5].

Hence the eigenvalues for (2) are given by (to the first order perturbation)

$$E_n = -\frac{G^2}{4(L+1+n_r)^2} + \langle \psi(r) | \frac{H}{r+z^2} | \psi(r) \rangle. \quad (6)$$

In order to compare our results with those of Znojil we take

$$F = -\frac{3}{16}, \quad z^2 = 1.$$

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Then (3) gives $L(L+1) = l(l+1) - 3/16$. Now

$$\langle \psi(r) | \frac{H}{r+z^2} | \psi(r) \rangle = \langle \psi(r) | H \sum_n (-1)^n r^n | \psi(r) \rangle \quad (7)$$

(taking $z^2 = 1$ and expanding $(1+r)^{-1}$ in a power series)

$$\begin{aligned} & \left(-\frac{G}{L+1+n_r} \right)^{2L+3} (n_r)! \\ &= \frac{(n_r)!}{(2L+2+2n_r)[\Gamma(n_r+2L+2)]^3} \\ & \cdot \sum_{n=0}^{\infty} (-1)^n \int_0^{\infty} H r^{2L+2+n} \exp \left\{ \frac{2Gr}{2L+2+2n_r} \right\} \\ & \cdot \left\{ L_{n_r}^{2L+1} \left(-\frac{Gr}{L+1+n_r} \right) \right\}^2 dr \\ &= \frac{(n_r)! H}{(2L+2+2n_r)[\Gamma(n_r+2L+2)]^3} \sum_n (-1)^n \\ & \cdot \int_0^{\infty} \left(\frac{L+1+n_r}{G'} \right)^n z^{2L+2+n} e^{-z} \{ L_{n_r}^{2L+1}(z) \}^2 dz, \\ & \left(G' = -G > 0 \text{ and } z = \frac{G'r}{L+1+n_r} \right) \\ &= \frac{H(n_r)! [(n+1)!]^2}{(2L+2+2n_r)[\Gamma(n_r+2L+2)]} \\ & \cdot \sum_n \sum_{\sigma} (-1)^n \left(\frac{L+1+n_r}{G'} \right)^n \\ & \cdot \frac{(-1)^{2n_r} \Gamma(2L+3+n+\sigma)}{(\sigma)! [(n_r-\sigma)!]^2 [(\sigma+n+1-n_r)!]^2}, \quad (8) \end{aligned}$$

where [5] σ takes on all integral values larger than $n_r - n - 2$ and smaller than $n_r + 1$.

For $n_r = 0$ and $n_r = 1$, (8) gives the following two equations:

$$\begin{aligned} \langle \psi(r) | H \sum_n (-1)^n r^n | \psi(r) \rangle &= \frac{H}{(2L+2) \Gamma(2L+2)} \\ & \cdot \sum_n (-1)^n \left(\frac{L+1}{G'} \right)^n \Gamma(2L+n+3) \quad (\text{for } n_r=0) \quad (9) \end{aligned}$$

and

$$\begin{aligned} \langle \psi(r) | H \sum_n (-1)^n r^n | \psi(r) \rangle &= \frac{H}{(2L+4) \Gamma(2L+3)} \\ & \cdot \sum_n (-1)^n \left(\frac{L+2}{G'} \right)^n \{ \Gamma(2L+n+5) \\ & - 4(L+1) \Gamma(2L+n+4) \\ & + 4(L+1)^2 \Gamma(2L+n+3) \} \quad (\text{for } n_r=1). \quad (10) \end{aligned}$$

Summation over n in (9) and (10) can be done by the method of Borel after Popov et al. [3]. For the sake of completeness we quote the result.

Let $f(z)$ be a function represented by an asymptotic series

$$f(z) = \sum_{k=k_0}^{\infty} a_k (-z)^k. \quad (11)$$

If the asymptotic representation of a_k is of the form

$$a_k = \frac{(k\alpha)!}{k!} a^k \sum_{m=0}^{\infty} C_m (k+\beta-m)!, \quad (12)$$

then the sum of the series (11) is

$$\begin{aligned} f(z) &= (az)^{-(\beta+1)} e^{1/az} \sum_{m=0}^{\infty} (\beta-m)! C_m (az)^m \\ & \cdot F(az, \alpha, m-\beta), \quad (13) \end{aligned}$$

where

$$F(az, \alpha, \beta) = x^{-\beta} \int_1^{\infty} e^{-t/x} [(t-1)^{\alpha} + 1]^{\beta-1} dt. \quad (14)$$

Using these formulas we obtain from (9) and (10).

$$\begin{aligned} \langle \psi(r) | H \sum_n (-1)^n r^n | \psi(r) \rangle &= \frac{H}{(2L+2) \Gamma(2L+2)} \\ & \cdot \left[\left(\frac{G'}{L+1} \right)^{(2L+3)} \exp \{ G'/(L+1) \} \Gamma(2L+3) \right. \\ & \cdot \Gamma \left(-2L-2; \frac{G'}{L+1} \right) \left. \right] \quad (\text{for } n_r=0), \quad (15) \end{aligned}$$

and

$$\begin{aligned} \langle \psi(r) | H \sum_n (-1)^n r^n | \psi(r) \rangle &= \frac{H}{(2L+4) \Gamma(2L+3)} \\ & \cdot \left[\left(\frac{G'}{L+2} \right)^{2L+5} \exp \{ G'/(L+2) \} \Gamma(2L+5) \right. \\ & \cdot \Gamma \left(-2L-4; \frac{G'}{L+2} \right) \left. \right] - \frac{4H(L+1)}{(2L+4) \Gamma(2L+3)} \\ & \cdot \left[\left(\frac{G'}{L+2} \right)^{(2L+4)} \exp \{ G'/(L+2) \} \Gamma(2L+4) \right. \\ & \cdot \Gamma \left(-2L-3; \frac{G'}{L+2} \right) \left. \right] + \frac{4H(L+1)^2}{(2L+4) \Gamma(2L+3)} \\ & \cdot \left[\left(\frac{G'}{L+2} \right)^{(2L+3)} \exp \{ G'/(L+2) \} \Gamma(2L+3) \right. \\ & \cdot \Gamma \left(-2L-2; \frac{G'}{L+2} \right) \left. \right] \quad (\text{for } n_r=1). \quad (16) \end{aligned}$$

Table 1. Bound state energies for different values of G and $H = 0.005$ ($l = 0$).

G	E_n	E_n^*
-0.0524404	-0.0099846	-0.01
-0.0279575	-0.0024830	-0.0025
-0.1540186	-0.00999	-0.01
-0.0794035	-0.00249	-0.0025
-0.01984185	-0.00009	-0.0001
-0.2539023	-0.00910	-0.01
-0.1291448	-0.00250	-0.0025
-0.02953019	-0.0001	-0.0001

* Denotes the values given by Znojil. Also for $H = 0.5$ (note a misprint in Table I of [1]) and $G = -0.3618325$ our first order formula reproduces the numerical results given by Znojil. This is not surprising because the Borel summation method in fact solves the integration problem exactly. This is shown in the Appendix where we obtain a recurrence relation for the integral $\int_0^\infty \frac{x^k e^{-bx}}{1+x} dx$ and compare it with our formula.

In deriving (15) and (16) we have used $F(x, 1, \beta) = \Gamma(\beta, x^{-1})$, $\Gamma(\beta, x^{-1})$ being the incomplete Gamma function [5].

Equations (15) and (16) together with (6) give the energy eigenvalues for $n_r = 0$ and $n_r = 1$, respectively. We have calculated the eigenvalues numerically for some specific values of G and H in order to compare our results with those obtained by Znojil, using the accurate numerical results given by Bessis and Bessis [2] for the potential $V(x) = x^2 + \lambda x^2/(1+g x^2)$. The values are shown in Table 1.

3. Conclusion and discussion

We have obtained an exact first order formula for the bound states for the potential

$$V(r) = F/r^2 + G/r + H/(r + z^2).$$

For small H compared with G , this reproduces the numerical results quoted by Znojil. The Borel summation method is proved to be very convenient in the investigation of this type of modified Coulomb potentials.

4. Appendix

The crucial integrals in evaluating the rhs of (6) are of the following type

$$I_k = \int_0^\infty \frac{x^k e^{-bx}}{1+x} dx. \quad (A1)$$

When $k = 0$, this can be expressed in terms of an exponential function.

$$I_0 = \int_0^\infty \frac{e^{-bx}}{1+x} dx = e^b E_1(b) \quad (\text{see [6], p. 230}). \quad (A2)$$

Now I_k can be written as

$$\begin{aligned} I_k &= (-1)^k \frac{d^n}{db^n} (I_0) \\ &= (-1)^k \frac{d^n}{db^n} [e^b E_1(b)] \\ &= -(-1)^{k-1} \frac{d^{n-1}}{db^{n-1}} [e^b E_1(b)] + \frac{(k-1)!}{b^k} \\ &= -I_{k-1} + \frac{(k-1)!}{b^k}. \end{aligned} \quad (A3)$$

The last but one step was obtained using formula 5.1.27 on p. 230 of [6]. Compare this with similar recurrence relations obtained by Bessis and Bessis in [2].

Now the Borel summation method, as described in II of the text, gives the following formula for I_k :

$$I_k = e^b \Gamma(k+1) \Gamma(-k, b). \quad (A4)$$

For $k = 0$:

$$I_0 = e^b E_1(b), \quad (A5)$$

which is identical with (A2). In deriving (A5) we have used formula 5.1.45 of [6].

Now using the recurrence relation for the incomplete gamma function, viz.

$$\Gamma(-k, b) = -\frac{\Gamma(-k+1, b)}{k} + \frac{1}{k} b^{-k} e^{-b} \quad (A6)$$

(see p. 262, [6]), it can be shown easily from (A4) that

$$I_k = -I_{k-1} + \frac{(k-1)!}{b^k}, \quad (A7)$$

which is identical with (A3).

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